The use of coarse-scale models in uncertainty quantification

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Introduction

- Dynamic data integration in subsurface applications consists of integrating large-scale data (e.g., production data) in order to reduce uncertainity and achieve realistic sampling of subsurface properties.
- Production data (usually measured with some precision) describes an integrated response (an average over the inter-well distance). Trying to obtain the permeability (hydraulic conductivity) samples based on this integrated response is an ill-posed problem.
- The problem reduces to sampling from a complicated distribition involving the solutions of coupled nonlinear partial differential equations.
- Metropolis-Hasting Markov chain Monte Carlo (MCMC) methods can be used as an umbrella sampling method. MCMC used in a straightforward way is very CPU demanding.
- We propose and analyze approaches for efficient sampling which employ spatial multi-scale models.

Prototypical model

We consider two-phase flow in a reservoir under the assumption that the displacement is dominated by viscous effects.

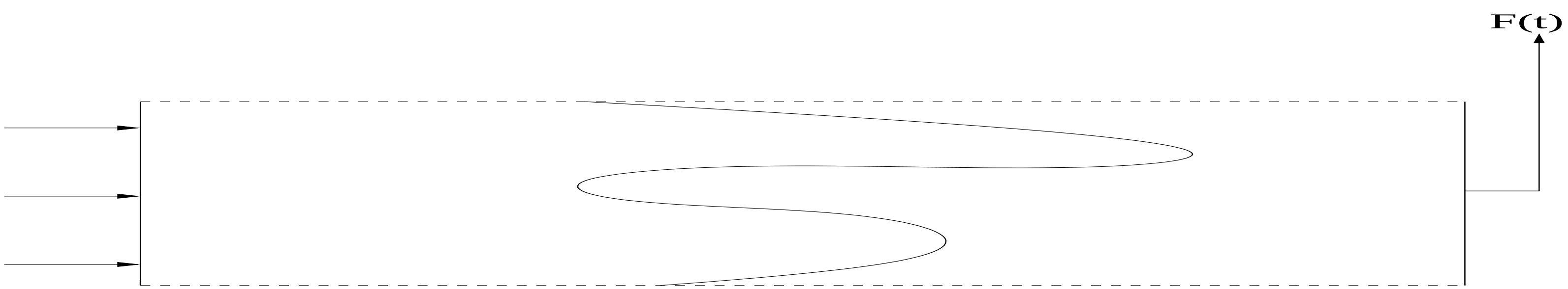
$$v_j = -\frac{k_{rj}(S)}{\mu_j} k \cdot \nabla p, \quad j = w, o$$

$$\nabla \cdot (\lambda(S) k \nabla p) = h,$$

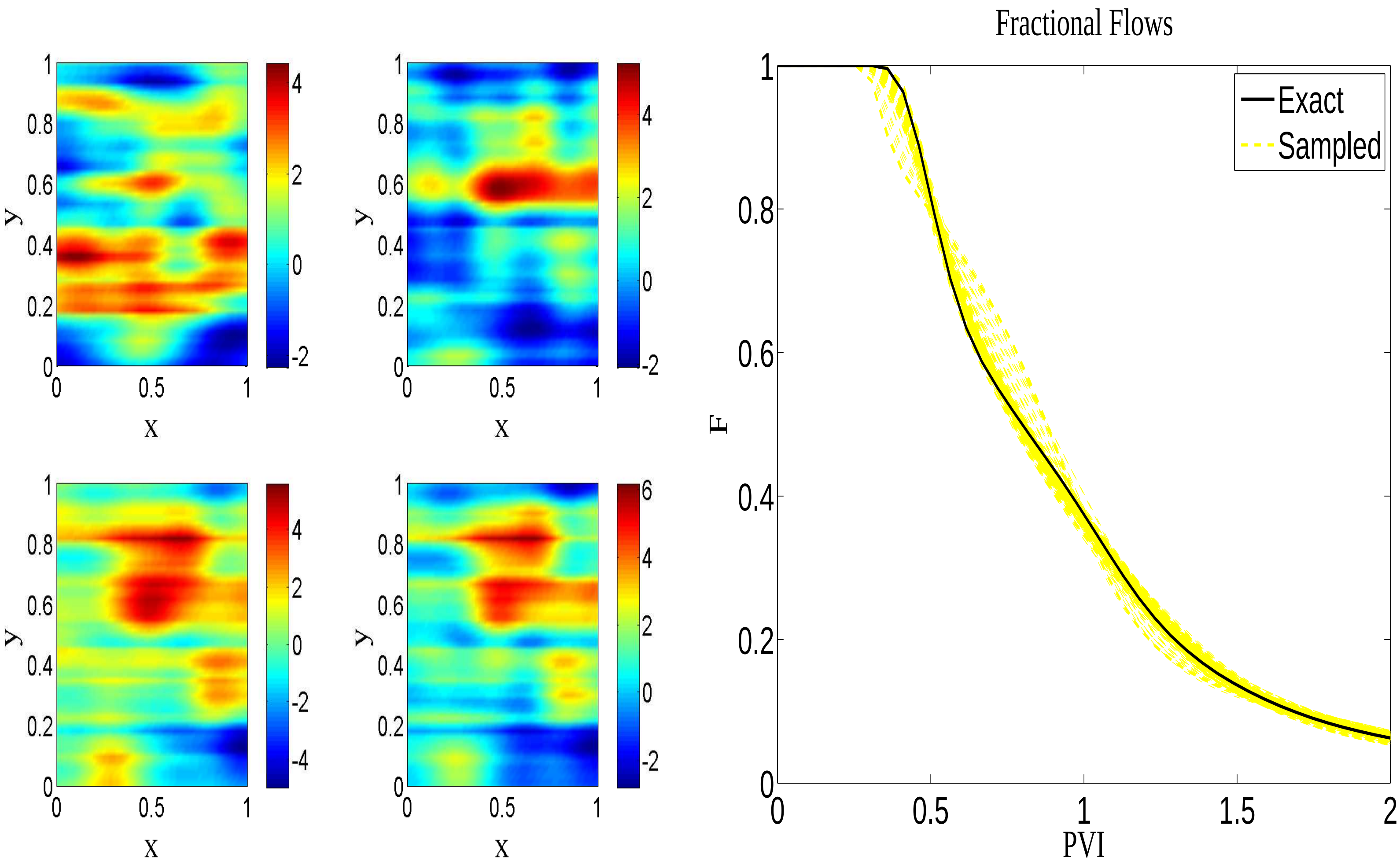
$$\frac{\partial S}{\partial t} + v \cdot \nabla f(S) = 0, \; v = -\lambda(S) k \nabla p.$$

Measure coarse-scale data:

$$F(t) = \frac{\int_{out} v f(S) dl}{\int_{out} v dl}$$



Illustration



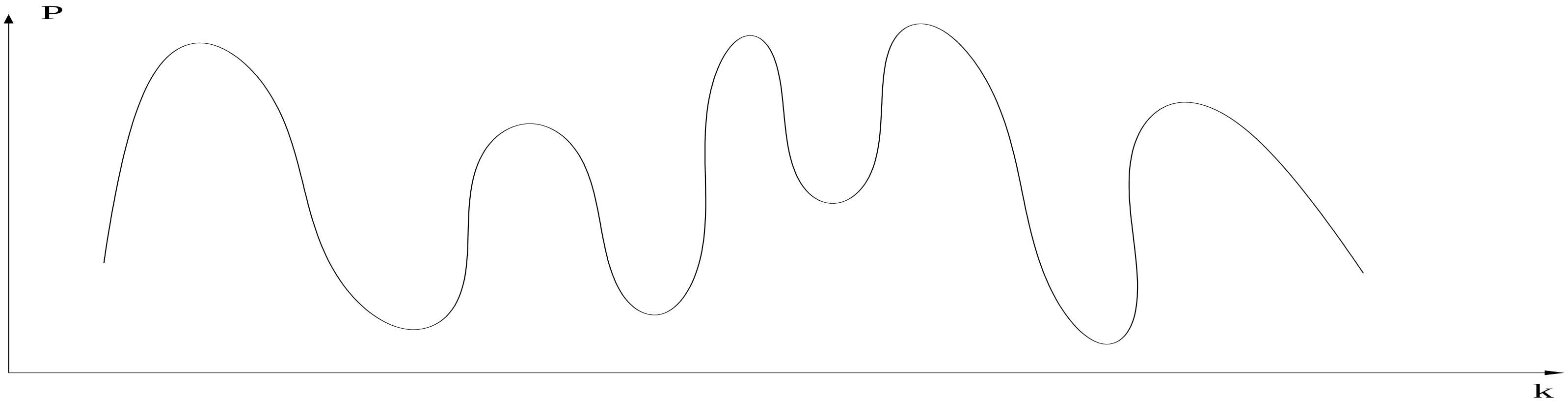
Problem setting

- Given the fractional flow information (coarse-scale data) $F(t)$ and some precision, we would like to sample k from $P(k|F)$.
- From Bayes theorem
$$P(k|F) \propto P(F|k)P(k).$$
- Here $P(k)$ is the prior information, $P(F|k)$ is the likelihood and assumed given by $P(F|k) = \exp(-\frac{\|F_k(t)-F^{obs}(t)\|^2}{\sigma_f^2})$.
- Typical prior can be $P(k) = \exp(-\frac{\|k-k_{obs}\|^2}{\sigma_k^2})$, where k_{obs} is a coarse-scale permeability. Thus, the posterior distribution is

$$P(k|F) \propto \exp(-\frac{\|F_k(t) - F^{obs}(t)\|^2}{\sigma_f^2}) \exp(-\frac{\|k - k_{obs}\|^2}{\sigma_k^2}).$$

Difficulties

- $\pi(k) = P(k|F)$ can be multi-modal and high dimensional.
- $\pi(k) = P(k|F)$ is not given analytically and involves the solution of nonlinear pde system.



Metropolis-Hastings MCMC

Algorithm (Metropolis-Hastings MCMC)

- Step 1. At k_n generate k from $q(k|k_n)$.
- Step 2. Accept k as a sample with probability

$$p(k_n, k) = \min\left(1, \frac{q(k_n|k)\pi(k)}{q(k|k_n)\pi(k_n)}\right),$$

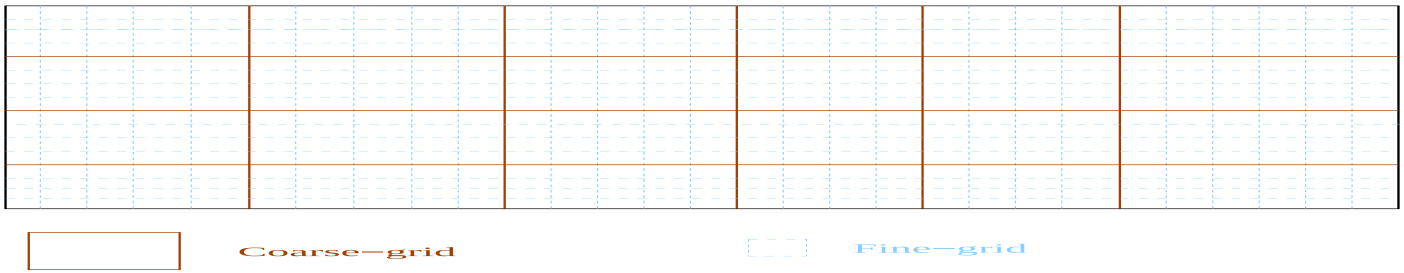
i.e. $k_{n+1} = k$ with probability $p(k_n, k)$, and $k_{n+1} = k_n$ with probability $1 - p(k_n, k)$.

Here $\pi(k)$ is the distribution we would like to sample.

- Direct (full) MCMC simulations are usually prohibitively expensive, because each proposal requires a fine-scale computation.
- We propose an algorithm, where the proposal distribution is modified using coarse-scale spatial models.

Coarse-scale spatial models

- An upscaled model is a representation of the fine-scale model on a coarse grid.
- In the single-phase upscaling procedures, the coarse-scale equations are of the same form, except the media properties are upscaled (i.e., k is replaced by k^*).
- We employ multiscale finite element methods as a single-phase upscaling technique. Multiscale methods, as traditional upscaling techniques, pre-compute effective parameters (basis functions) that are repeatedly used for different boundary condition, sources and mobilities.
- The pressure equation is upscaled using multiscale finite volume method and coarse-scale velocity field is calculated and used for solving the saturation equation. Basis functions are constructed only at time zero.
- This provides a very inexpensive approximation for the solution.



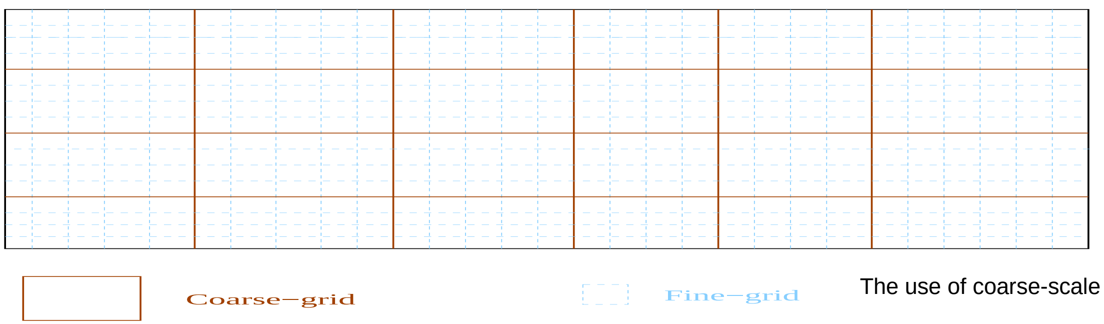
Multiscale methods

Consider $div(k(x)\nabla p) = f$.

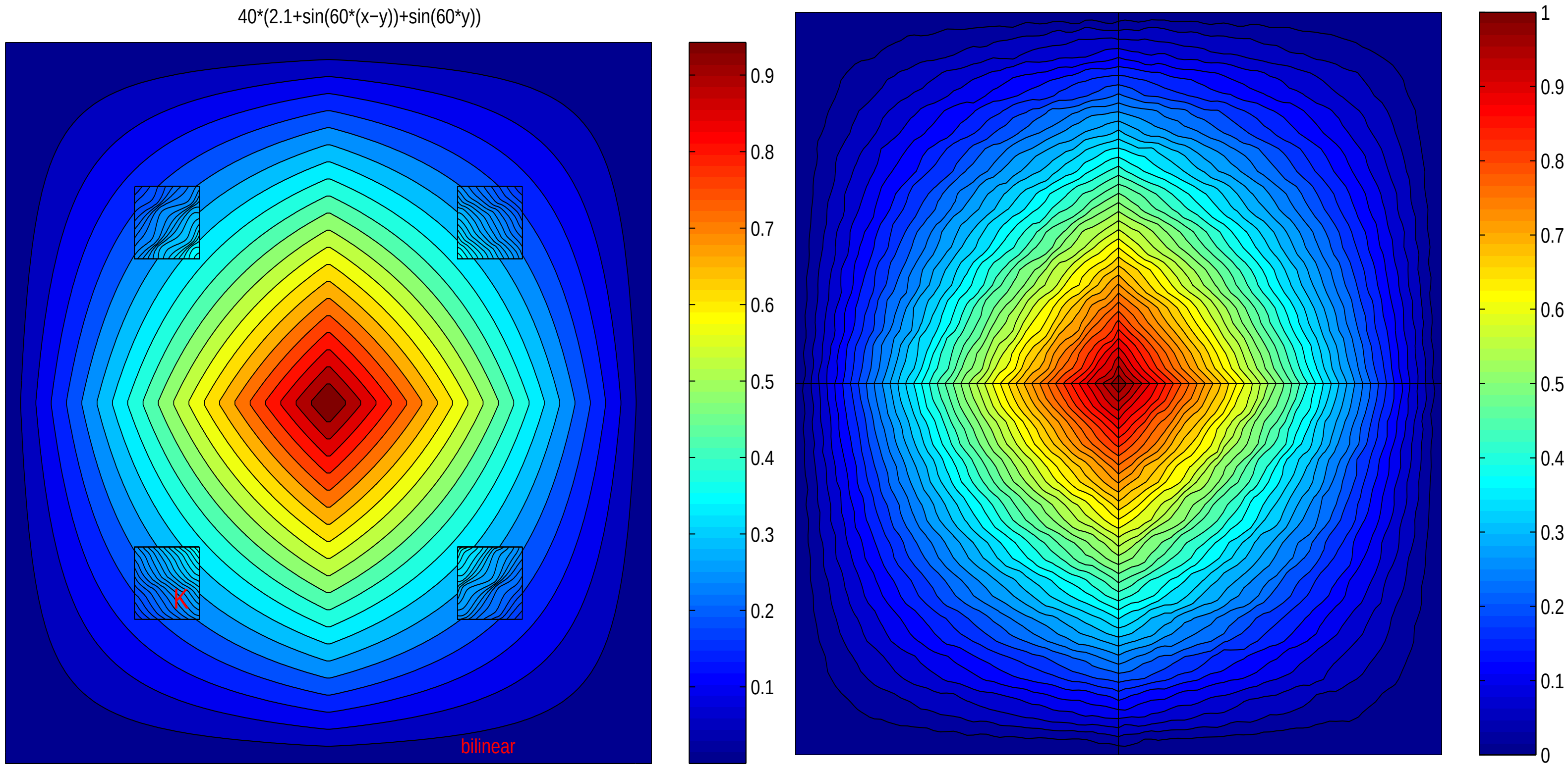
- Our goal is to solve this equation on a coarse grid of size h.
- Basis functions are constructed by solving the leading order homogeneous equation in an element K (coarse grid or RVE)

$$div(k(x)\nabla \phi^i) = 0 \quad \text{in} \quad K$$

- Boundary conditions are very important for accuracy of subgrid capturing error. Choices: (1) local boundary conditions (the information only within the target coarse block is taken into account); (2) oversampling (the information in slightly larger than the target coarse block domain is taken into account).
- It is known that the local approaches suffer from the resonance errors expressed as the ratio *characterstic length scale/coarse mesh size*. Limited global information (important global information) can be used to remove the resonance errors.



Basis functions



$\phi^i = \phi_0^i$ on ∂K, where ϕ_0^i are standard bilinear basis functions.

Stochastic multiscale finite element methods

- Multiscale methods using limited global information rely on the assumption that the solution smootly depends on some global fields in two-phase flow simulations

$$\|p - G(p_1, ..., p_N)\|_{H^1} \leq \delta,$$

  where δ is small. This holds for two-phase flows.
- One can construct multiscale (velocity) basis functions such that the obtained mixed MsFEM converges with the rate $C(\delta + h^\alpha)$.
- In stochastic MsFEM, selected realizations are used to construct bassi functions. Then, for any realization, the solution can be projected into this finite dimensional space.
- Solve the pressure equation on the coarse-grid with fixed set of basis functions and solve the saturation equation on the coarse-grid.
- Methods are not restricted to box grids and handle corner-point grids.

Langevin Algorithms

An important type of proposal distribution can be derived from the Langevin diffusion. The Langevin diffusion is defined by the stochastic differential equation

$$dk(\tau) = \frac{1}{2}\nabla \log \pi(k(\tau))d\tau + dW_\tau,$$

where W_τ is the standard Brownian motion vector with independent components. The solutions of this stochastic differential equation are from $\pi(k)$.
A discretization of the equation,

$$k_{n+1} = k_n + \frac{\Delta\tau}{2}\nabla \log \pi(k_n) + \sqrt{\Delta\tau}\epsilon_n,$$

where ϵ_n are independent standard normal distributions.
The proposal is chosen to be

$$Y = k_n + \frac{\Delta\tau}{2}\nabla \log \pi(k_n) + \sqrt{\Delta\tau}\epsilon_n,$$

Langevin Algorithms

The transition distribution of the proposal is

$$q(Y|k_n) \propto \exp\left(-\frac{\|Y - k_n - \frac{\Delta\tau}{2}\nabla \log \pi(k_n)\|^2}{2\Delta\tau}\right),$$

$$q(k_n|Y) \propto \exp\left(-\frac{\|k_n - Y - \frac{\Delta\tau}{2}\nabla \log \pi(Y)\|^2}{2\Delta\tau}\right).$$

The reasons for using Langevin:

- Pde's describing the physical model allow us to compute the gradients.
- The use of gradients is common in "stochastic" subsurface applications, e.g., Randomized Maximum Likelihood (RML). This approach samples the measurement data and the prior information independently and then minimize the posterior functional with these samples.
- The use of Langevin proposals usually yields higher mixing rates compared to e.g., random walk sampler.

Preconditioned coarse-gradient Langevin algorithm

The main idea: (1) use coarse-scale simulations to compute the gradient and make a proposal; (2) run the coarse-scale simulation code and check the "appropriateness" of the sample; (3) run the "fine-scale" simulation.

- Step 1. At k_n, generate a trial proposal Y from the coarse Langevin distribution $q^*(Y|k_n)$.
- Step 2. Take the proposal k as

$$k = \begin{cases} Y \text{ with probability } g(k_n, Y), \\ k_n \text{ with probability } 1 - g(k_n, Y), \end{cases}$$

where

$$g(k_n, Y) = \min\left(1, \frac{q^*(k_n|Y)\pi^*(Y)}{q^*(Y|k_n)\pi^*(k_n)}\right).$$

- Step 3. Accept k as a sample with probability

$$\rho(k_n, k) = \min\left(1, \frac{Q(k_n|k)\pi(k)}{Q(k|k_n)\pi(k_n)}\right),$$

where Q is the effective proposal distribution.

Preconditioned coarse-gradient Langevin algorithm

- The transition distribution of the coarse-grid proposal is

$$q^*(Y|k_n) \propto \exp\left(-\frac{\|Y - k_n - \frac{\Delta\tau}{2}\nabla\log\pi^*(k_n)\|^2}{2\Delta\tau}\right),$$

$$q^*(k_n|Y) \propto \exp\left(-\frac{\|k_n - Y - \frac{\Delta\tau}{2}\nabla\log\pi^*(Y)\|^2}{2\Delta\tau}\right).$$

Convergence of modified Markov Chain

Denote

$$\mathcal{E} = \{k;\ \pi(k) > [0]\},$$

$$\mathcal{E}^* = \{k;\ \pi^*(k) > [0]\},$$

$$\mathcal{D} = \{k;\ q(k|k_n) > [0] \text{ for some } k_n \in \mathcal{E}\},$$

To sample from $\pi(k)$ correctly, it is necessary that $\mathcal{E} \subseteq \mathcal{E}^*$. Otherwise, there will exist a subset $A \subset (\mathcal{E} \setminus \mathcal{E}^*)$ such that

$$\pi(A) = \int_A \pi(x)dx > 0 \qquad \text{and} \qquad \pi^*(A) = \int_A \pi^*(x)dx = 0.$$

As a result, the chain $\{k_n\}$ will never visit (sample from) A since the element of A will never be accepted for fine-scale run in Step 2. For the same reason, we should require that $\mathcal{E} \subseteq \Omega$.

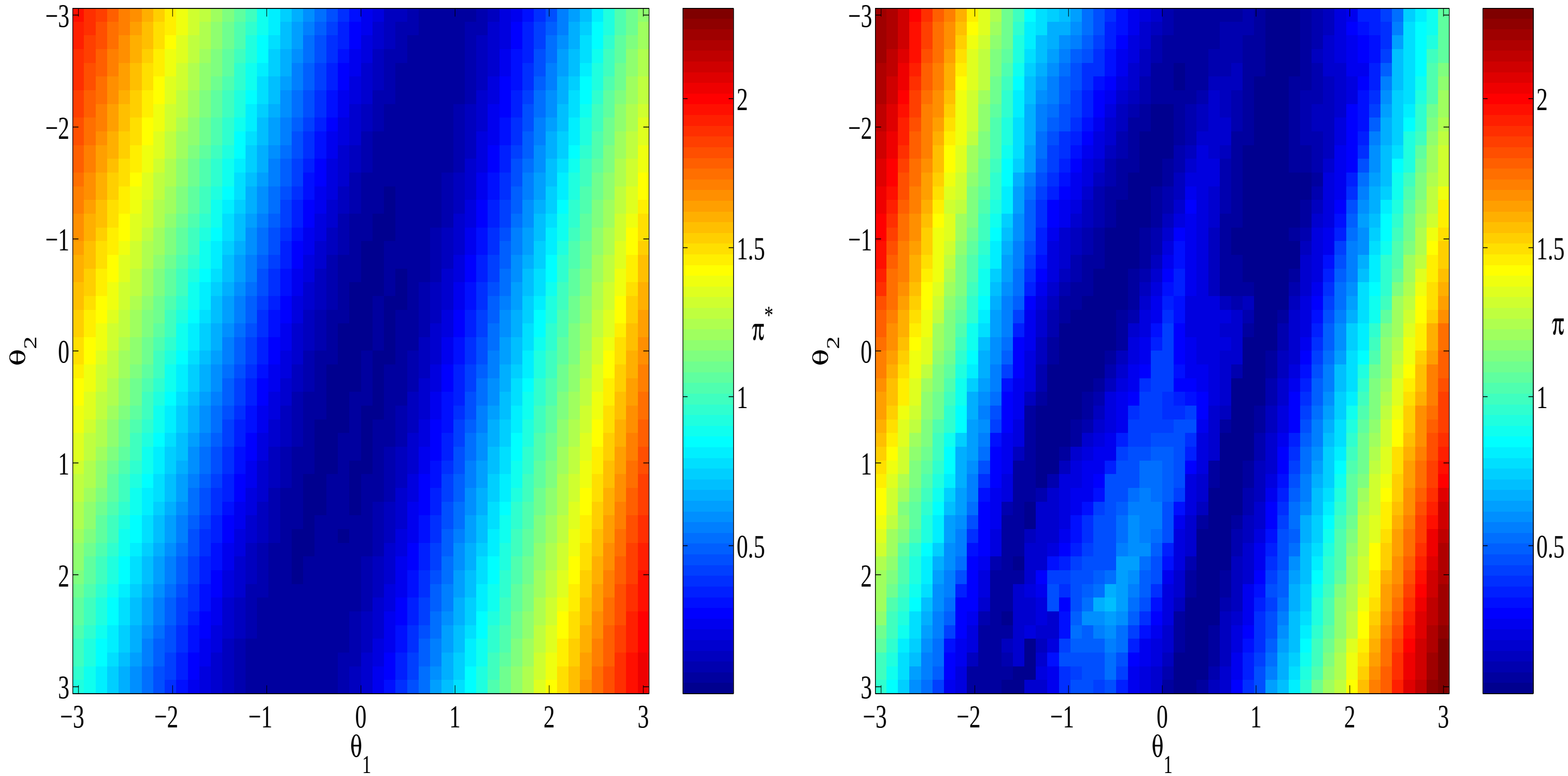
Numerical setting

- We consider log-normal permeability fields $k(x) = \exp(Y(x))$, where $Y(x)$ is prescribed with a covariance matrix (e.g., normal or exponential).
- The permeability field is parameterized via Karhunen-Loève Expansion

$$Y(x,\omega) = \sum_{k=1}^{\infty} \sqrt{\lambda_k}\theta_k(\omega)\phi_k(x),$$

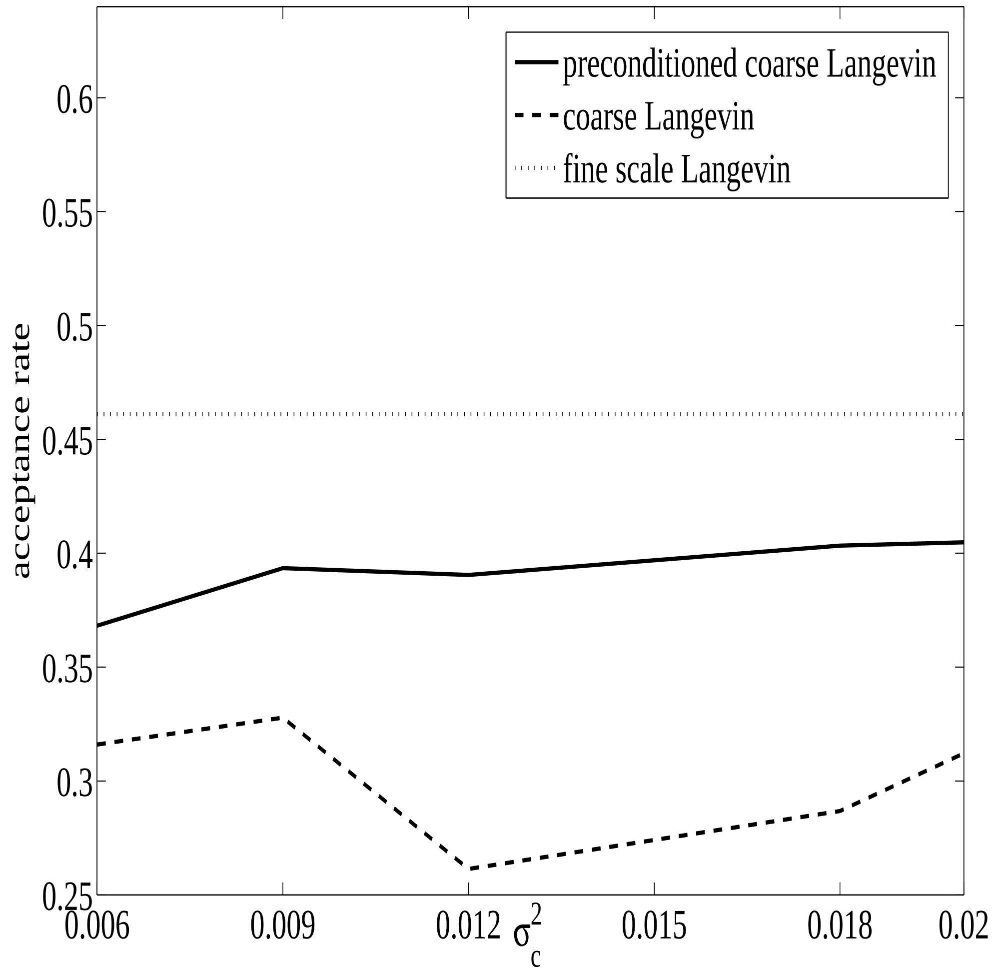
  where $E(\theta_k) = 0$, $E(\theta_i\theta_j) = \delta_{ij}$, λ_k and $\phi_k(x)$ are eigenvalues and eigenvectors of covariance matrix.
- First step parameter reduction is performed by neglecting “small” eigenvalues.
- The permeability field can be conditioned at well locations.

Numerical Results



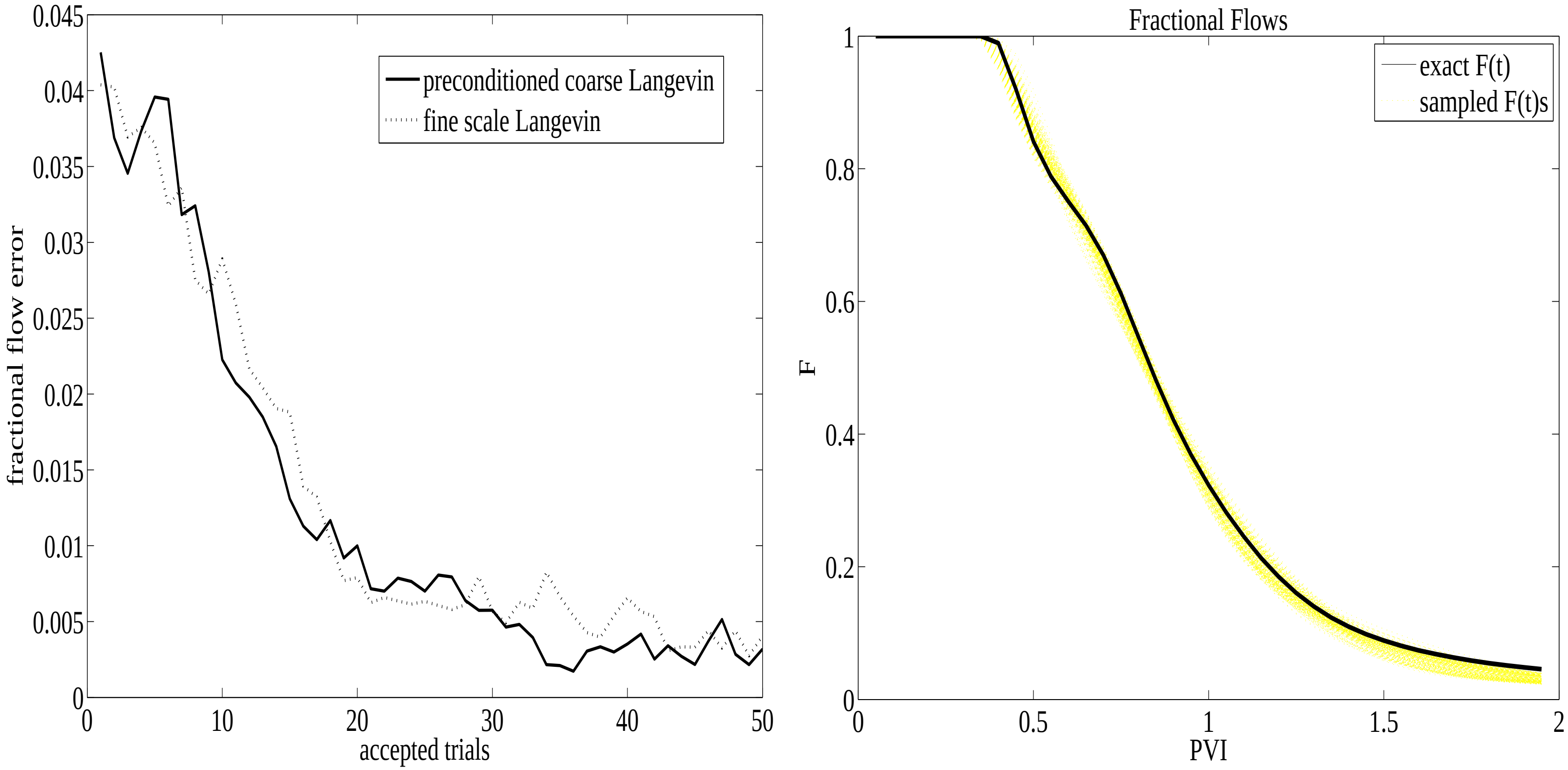
Left: Coarse-scale response surface π^* restricted to a 2-D hyperplane. Right: Fine-scale response surface π restricted to the same 2-D hyperplane.

Numerical results



Acceptance rate comparison, $\delta = 0.1$.

Numerical results



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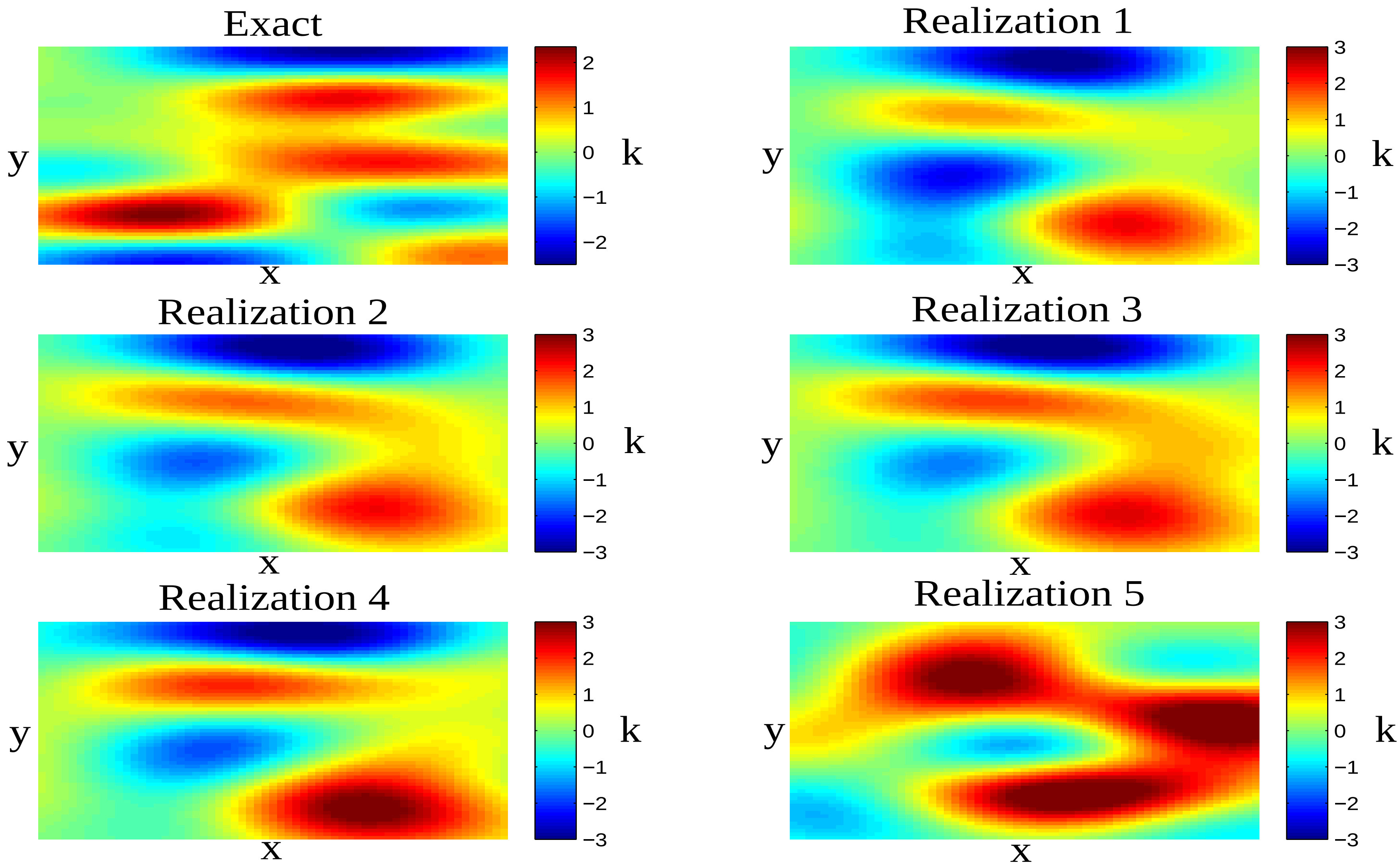
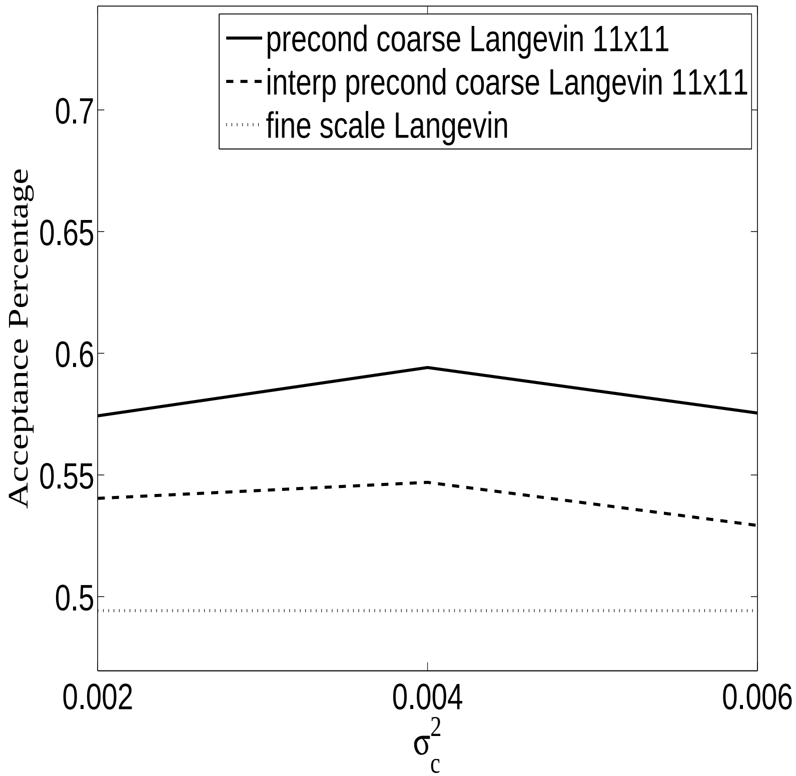
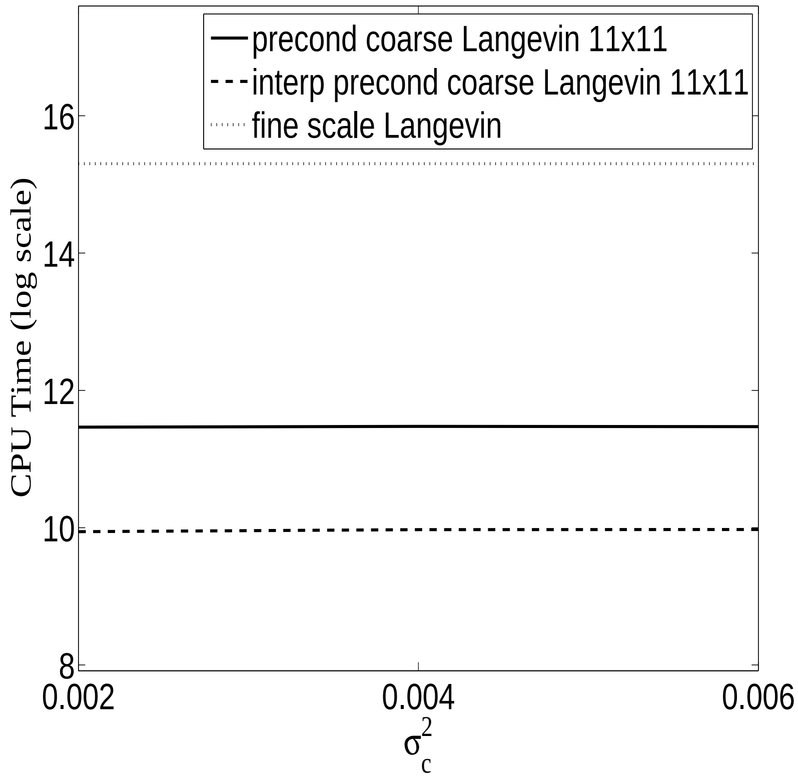


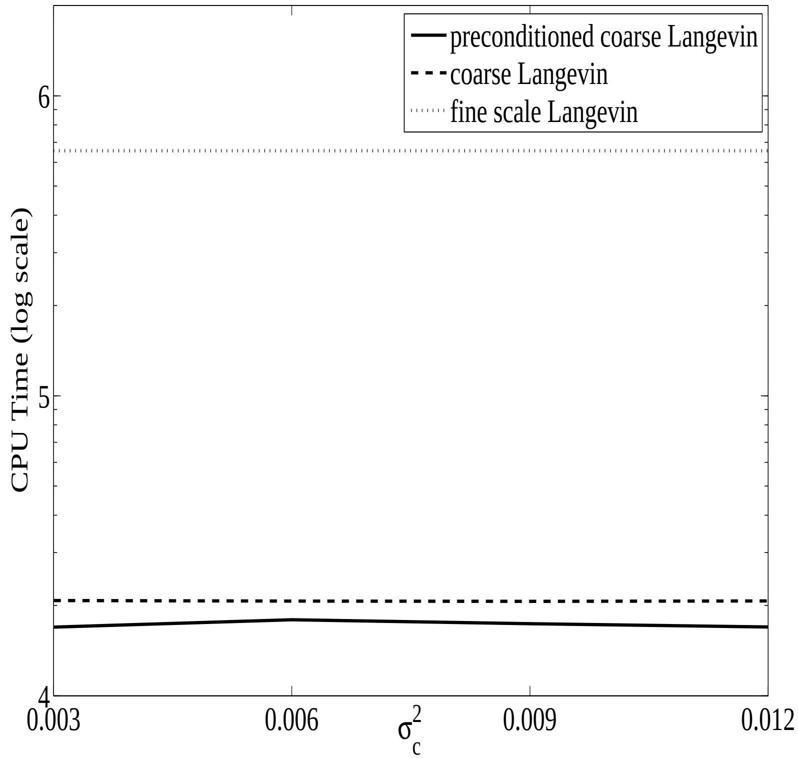
Numerical Results





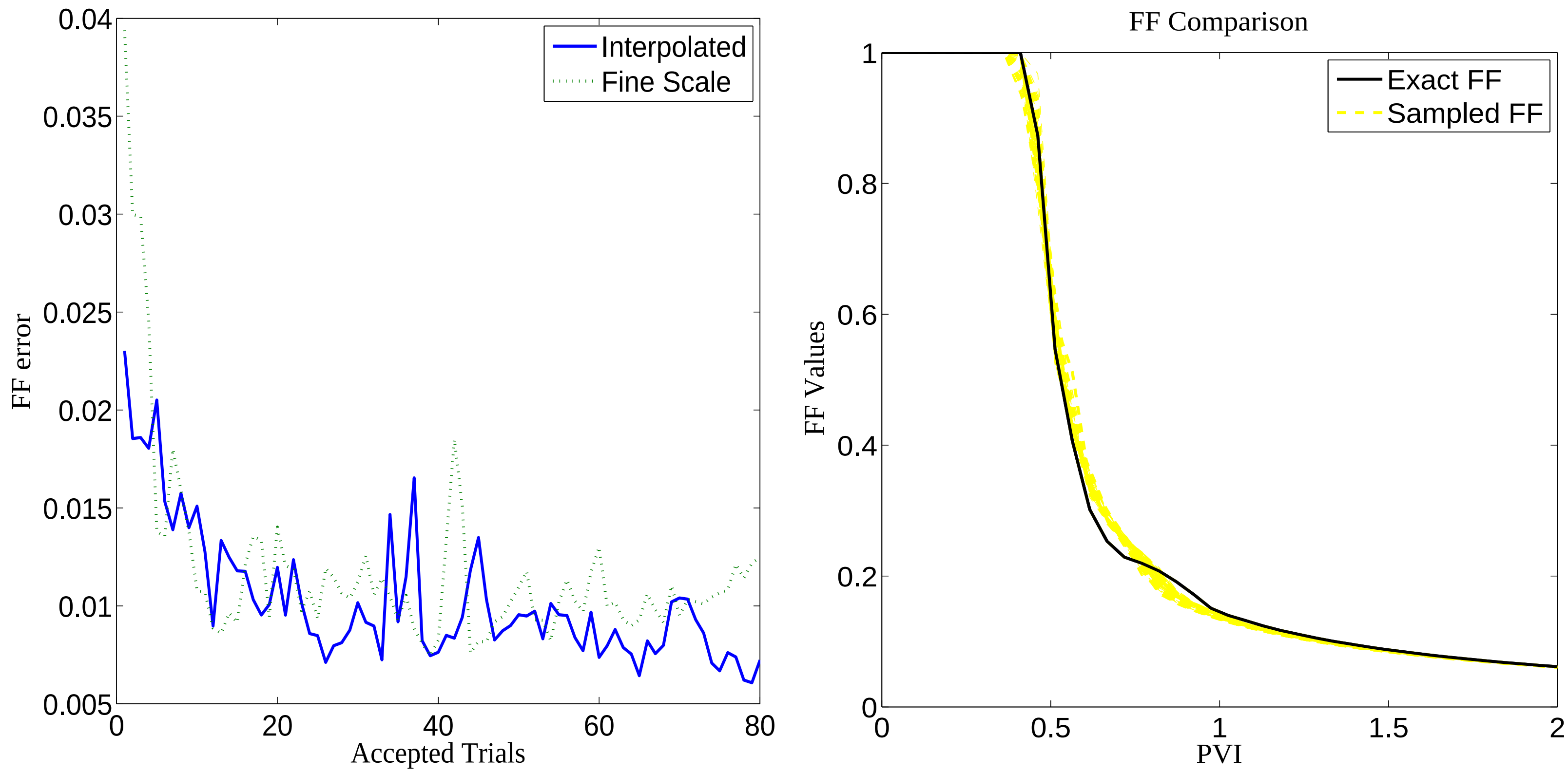
Left: Acceptance rate comparison. Right: Natural log of CPU time (seconds) comparison. In each plot $\delta = 0.05$ and $\sigma_f^2 = 0.002$.

Numerical Results



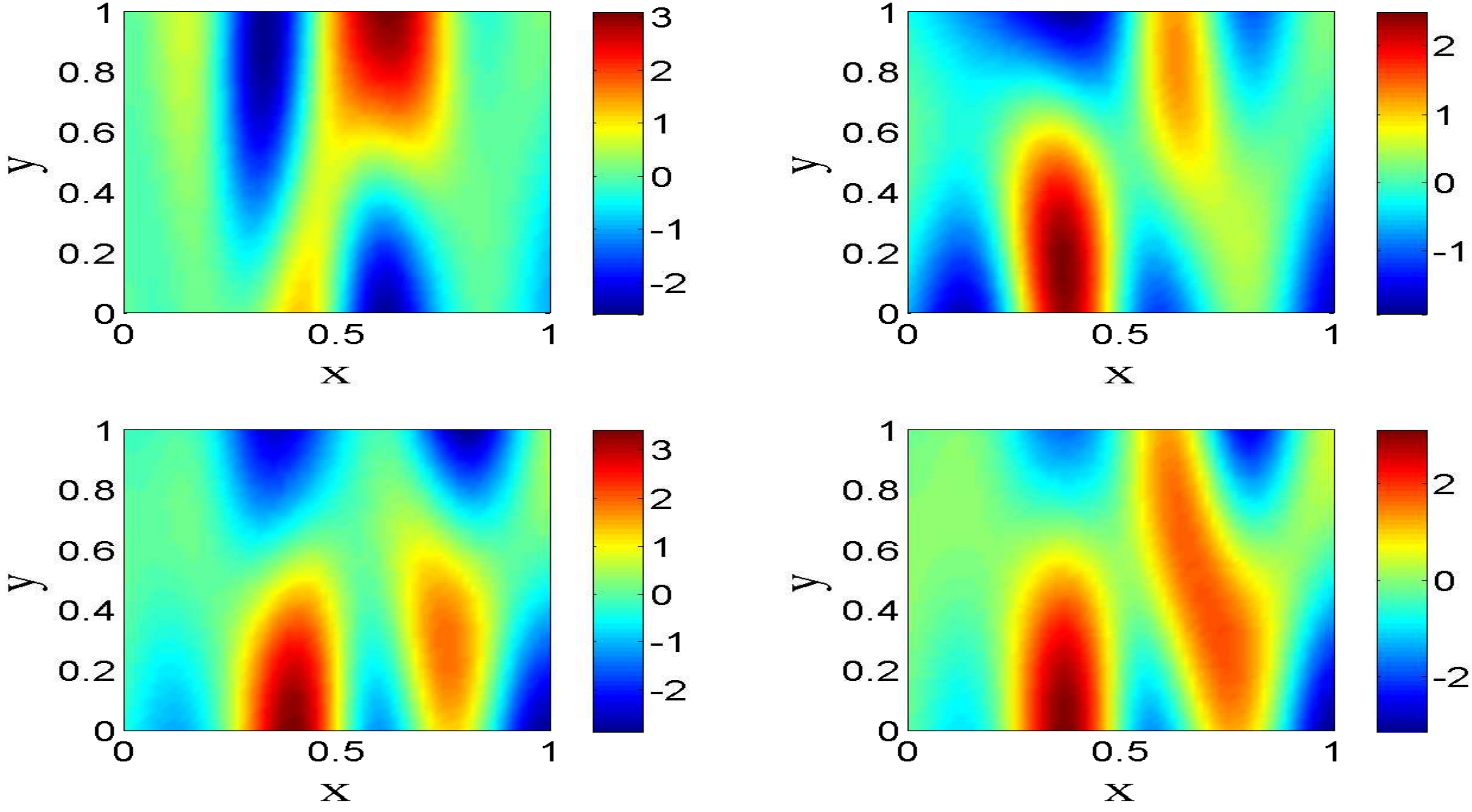
CPU times (seconds) for Langevin algorithms. $\sigma_f^2 = 0.003$, $\delta = 0.05$, 7×7 coarse-grid.

Numerical Results



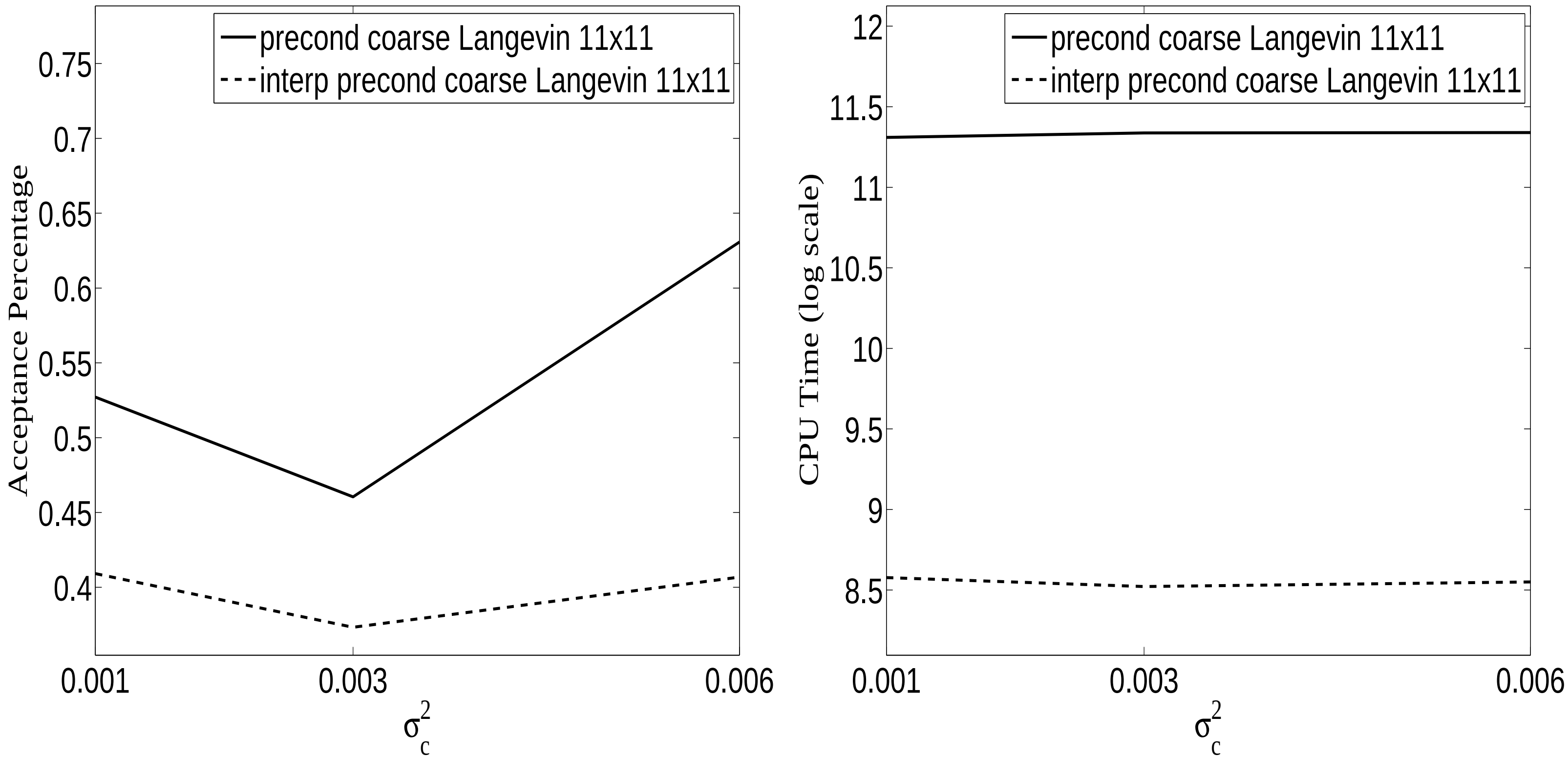
Left: The fractional flow errors for the fine Langevin algorithm compared with interpolated Langevin algorithm. Right: The fractional flows of sampled realizations and the reference fractional flow. In these numerical tests, $\delta = 0.05$ and $\sigma_f^2 = 0.002$.

Numerical Results



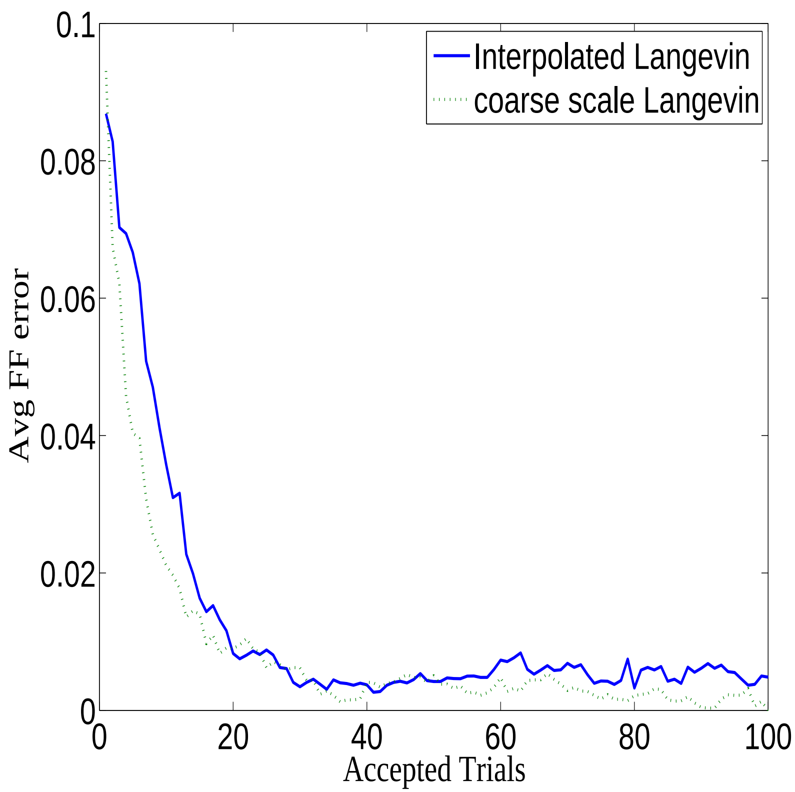
Upper left plot is the reference permeability. The other three plots are examples of accepted permeability realizations.

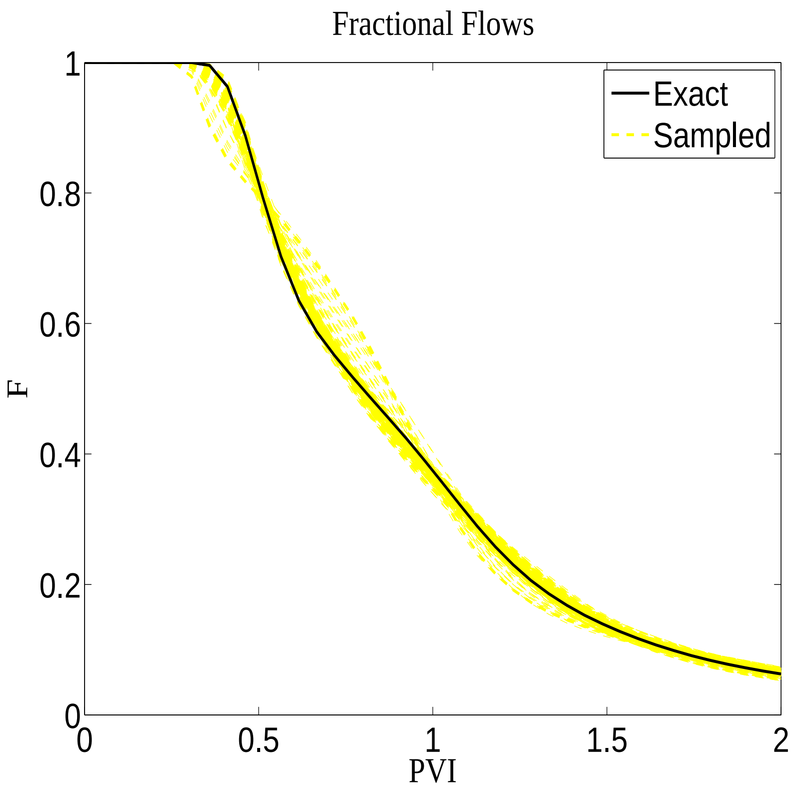
Numerical Results



Left: Acceptance rate comparison. Right: Natural log of CPU time (seconds) comparison. In each plot we use $\delta = 0.05$ and $\sigma_f^2 = 0.001$.

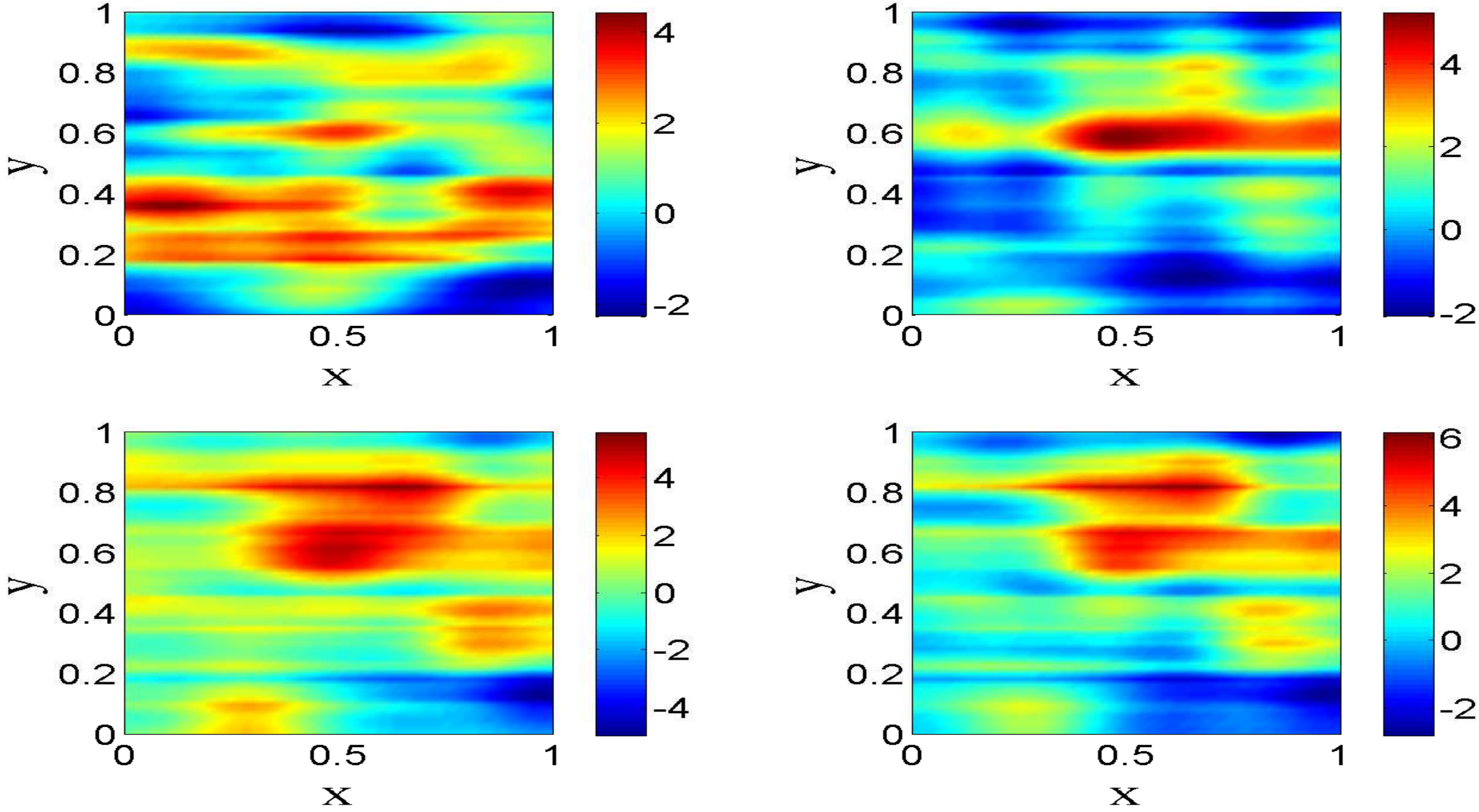
Numerical Results





Left: The fractional flow errors for coarse Langevin compared with interpolated Langevin. Right: The fractional flows of sampled realizations and the reference fractional flow. In these numerical tests, $\delta = 0.05$, $\sigma_f^2 = 0.001$.

Numerical results



Upper left plot is the reference permeability. The other three plots are examples of accepted permeability realizations.

Conclusions

- Direct sampling using MH MCMC approaches is expensive
- Inexpensive coarse-scale models can be used to precondition Langevin MH simulations.
- Coarse-scale simulations are based on multiscale finite element type methods.
- Multiscale basis functions can be constructed to represent an ensemble of permeability fields.
- Numerical results demonstrate CPU time can be reduced by two orders of magnitude.
- So far, we have used permeability priors which assume that the covariance structure of the permeability is known. We plan to use discontinuous priors, e.g., BPM (Bayesian Partition Method), in future.